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Quantum spin glass phase boundary in transverse field Ising systems

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Abstract : Here we study zero temperature quantum phase transition driven by the transverse field for random $\pm J$ Ising model on chain and square lattice. We present some analytical results for one dimension and some numerical results for very small square lattice under periodic boundary condition. The numerical results are obtained employing exact diagonalization technique following Lanczos method.

Keywords : Quantum phase transition, spin glasses, transverse Ising model, exact diagonalization.

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1. Introduction

The interest in the study of transverse Ising spin glass models was revived in early 1990 by the discovery of zero-temperature transition in dipolar Ising transverse field magnet $LiHo_xY_{1-x}F_4$ [1]. Proton glasses such as mixture of ferroelectric and anti-ferroelectric materials like $Rb_{(1-x)}(NH_4)_x(H_2P)_4$ [2] also provided earlier useful realizations of such quantum spin glasses.

These developments initiated extensive theoretical studies in quantum spin glass models. Ising model in transverse field has already been studied extensively in this context through analytical approaches using approximate renormalization techniques and real space renormalization group method, as well as using numerical methods like quantum Monte Carlo and exact diagonalization techniques [3]. Fairly extensive studies on the quantum spin glass phases have been made so far for transverse field Edward-Anderson model and Sherrington-Kirkpatrick model with random exchange distributions [3,4] and to some extent on quantum Heisenberg spin glass models [4]. In view of the rigorous developments in the study of two dimensional nearest neighbour Ising model with random $\pm J$ exchange interactions and the precise knowledge of location of the Nishimori line [5] in such classical spin glass model (driven by temperature), we consider here the quantum phase transition (at zero temperature) in the same $\pm J$ Ising model.

We have shown analytically that introduction of random $-J$ impurities cannot affect the zero temperature phase transition in one dimensional system as they can be transformed away. We have also compared and verified the result numerically for the small system size considered. For two dimensional systems, we present some priliminary results obtained for a square lattice using exact diagonalization results for very small system sizes following Lanczos technique [6]. Only the behaviours of configurationally averaged energy gap $\Delta = (E_1 - E_0)$ between the first excited state and the ground state and the second order response function $\chi = (\partial^2 E_0/\partial \Gamma^2)$, equivalent to specific heat, have been studied here. The variations of Δ and χ with respect to transverse field Γ

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have been obtained, and the phase boundary has been estimated from these results.

We work with a transverse Ising system, using only nearest neighbour interactions, whose Hamiltonian is given by

$$H = -\sum_{\langle i,j\rangle} J_{ij} S_i^z S_j^z - \Gamma \sum_{i=1}^{N} S_i^x \tag{1}$$

where the transverse field Γ is uniform through out the system and the nearest neighbour exchange constant J_{ij}'s are chosen randomly from the binary distribution

$$P(J_{ij}) = p\delta(J_{ij} + J) + (1 - p)\delta(J_{ij} - J). \tag{2}$$

Here, J is taken positive and p is thus the concentration of anti-ferromagnetic $-J$ bonds in the system.

2. Results in one dimensional system

Here, first we show analytically that in a one dimensional transverse Ising Hamiltonian with uniform J and Γ, if we replace some J bonds by $-J$ bonds randomly, then the resulting Hamiltonian can be gauge transformed back to one with uniform J, and hence the critical field remains unchanged with randomness concentration. Simillar result for one dimensional system with distributed J had been obtained earlier [7].

Let us take the one dimensional random bond tranverse Ising Hamiltonian

$$H = -\sum J_i S_i^z S_{i+1}^z - \sum \Gamma S_i^x \tag{3}$$

where the transverse field Γ is uniform throughout the system, and J_i's are randomly chosen from the same distribution as given in eq. (2). Since the J_i's have same magnitude J all through, and their randomness is only in their sign, we may write $J_i = J\mathrm{sgn}(J_i)$, and thus Hamiltonian (3) takes the form

$$H = -\sum_i \mathrm{sgn}(j_i) S_i^z S_{i+1}^z - \Gamma \sum_i S_i^x . \tag{4}$$

Now, let us define a new set of spin variables as below:

$$\tilde{S}_i^z = S_i^z \prod_{k=1}^{i-1} \mathrm{sgn}(J_k),$$

$$\tilde{S}_i^x = S_i^x,$$

$$\tilde{S}_i^y = S_i^y \prod_{k=1}^{i-1} \mathrm{sgn}(J_k).$$

It is easy to see that $\tilde{S}$'s satisfy the same commutation and anti-commutation relations as those of S's and hence will exhibit exactly the same dynamical behaviour. Now,

$$\tilde{S}_i^z \tilde{S}_{i+1}^z = S_i^z S_{i+1}^z \prod_{k=1}^{i-1} \mathrm{sgn}(J_k)^2 \ \mathrm{sgn}(j_i).$$

or

$$\tilde{S}_i^z \tilde{S}_{i+1}^z = S_i^z S_{i+1}^z \,\mathrm{sgn}(j_i),$$

since $[\mathrm{sgn}(J_k)]^2 = 1$. Thus in terms of new spin variables, Hamiltonian (4) becomes

$$H = -J \sum \tilde{S}_i^z \tilde{S}_{i+1}^z - \Gamma \sum \tilde{S}_i^x . \tag{5}$$

The above Hamiltonian describes the same random system in terms of new variables, and yet, as one can see, it has in itself no randomness at all. One can use Jordon-Wigner transformation in terms of $\tilde{S}$'s and see that here also quantum phase transition occurs only at $\Gamma \geq \Gamma_c (= J)$ as it occurs in a non-random Hamiltonian in S's. In Figure 1, we present some data computed for a chain of size $N = 9$, which shows that the gap Δ vanishes at $\Gamma_c \approx 1$ (the field being scaled by J). These data for $\Delta = E_1 - E_0$ is obtained from the computed average value of E_0 and E_1, each one averaged over about 10 configurations for $p \neq 0$. For infinite system, Δ is a linear function of Γ for $\Gamma > \Gamma_c$. In our case, linearity is observed at high values of Γ, and Γ_c is determined by backward linear extrapolation from the linear region. From the numerical data in Figure 1, we see that there is a slight variation

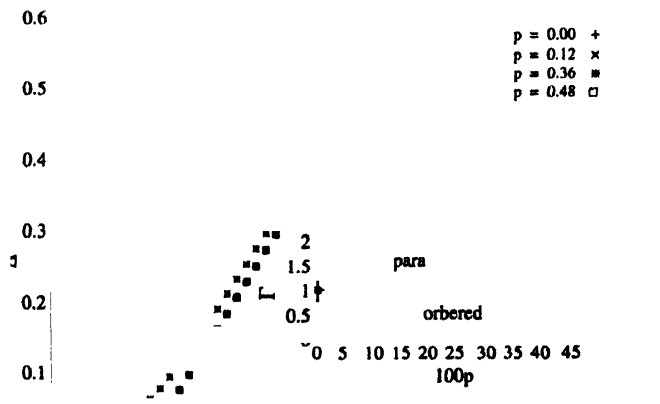

Figure 1. A numerical estimate of the energy gap Δ for a chain with $N = 9$. Phase boundary is obtained from the location of $\Delta(\Gamma) = 0$, and is shown in the inset.

of Γ_c with p (Γ_c varies between 0.9 and 1.0). This variation can be attributed to the very small size of the system. However, it may be noted that with even number of $-J$ bonds in the chain, with periodic boundary condition, there is no problem of incommensuration and $E_0(\Gamma)$ or $E_1(\Gamma)$ become strictly identical for such values of p. Similarly, in every case of odd number of $-J$ bonds in the chain, incommensuration problem always occurs for one spin only, rendering identical values (but different from the even $-J$ case) for $E_0(\Gamma)$ and $E_1(\Gamma)$ in all such cases.

3. Results for square lattice

We consider now the same system (represented by Hamiltonian (1)) on a square lattice of size 3 × 3 with periodic boundary condition. We again calculate the ground state and the first excited state energy E_0 and E_1 respectively as functions of the transverse field Γ, for different values of p. Each value of E_0 and E_1 is averaged over at least 10 configurations for each $p \neq 0$. Apart from Δ, we also calculate $\chi = \partial^2 E_0/\partial\Gamma^2$ and their variations with Γ as shown in Figures 2 and 3 respectively.

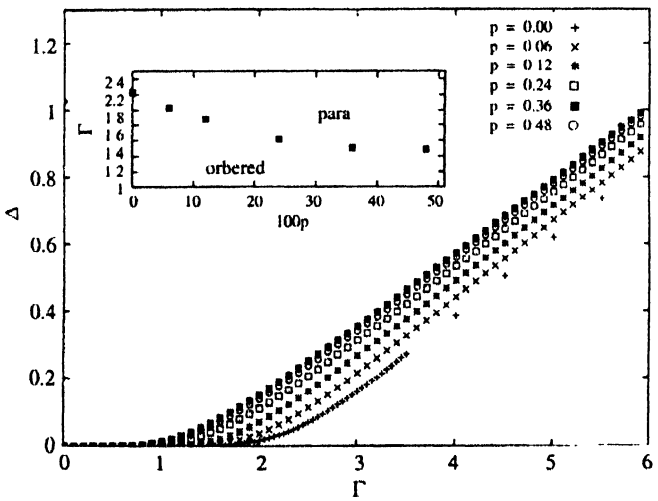

Figure 2. A numerical estimate of the configurational average of the energy gap Δ for a square lattice of size 3 × 3. Phase boundary obtained from $\Delta(\Gamma) = 0$ is outlined in the inset.

Our results here are severely constrained by the system size. The value of pur ferromagnetic critical field Γ_c (p = 0) is found here to be around 2.2, while the series results [3] or cluster algorithms [8] give the value to be around 3.0. This discrepancy is attributed to the smallness of our system size ($N = 3^2$). However, the qualitative behaviour of the order-disorder phase boundary (between ferro/spin glass and para) seems to be reasonable : $\Gamma_c(p)$ decreases with p initially, and then increases again as p approaches unity (pure antiferromagnet). The use of periodic boundary condition here (to avoid some numerical errors) also restricts the domain features and thereby affects our results. The absence of the knowledge of the ground-state wave function (and the correlation functions) in this method also forbids us to analyse the structure of the ordered phases.

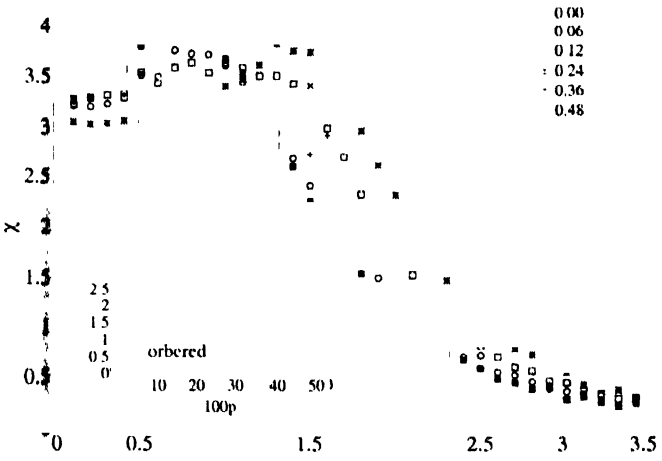

Figure 3. Variation of $\chi = \partial^2 E_0/\partial\Gamma^2$ with Γ. The transition point occurs at $\Gamma = \Gamma_c$ where χ diverges; for finite system, one gets only a peak in χ at $\Gamma = \Gamma_c(p)$ We have outlined the corresponding phase boundary in the inset.

Acknowledgments

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